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Universal Short-time Behaviour of the Dynamic Fully Frustrated XY Model*

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Abstract

With Monte Carlo methods we investigate the dynamic relaxation of the fully frustrated XY model in two dimensions below or at the Kosterlitz-Thouless phase transition temperature. Special attention is drawn to the sublattice structure of the dynamic evolution. Short-time scaling behaviour is found and universality is confirmed. The critical exponent θ is measured for different temperature and with different algorithms.

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I. INTRODUCTION

There has been a long history for the study of universal scaling behaviour for critical dynamics. It is well known that there exists a universal scaling form when dynamic systems almost reach equilibrium or in the long-time regime of the dynamic evolution. When a dynamic magnetic system has evolved for a sufficiently long time, the magnetization decays exponentially. The characteristic time scale for this regime is $t_\tau \sim \tau^{-\nu z}$ or $t_L \sim L^z$ with τ being the reduced temperature and L being the lattice size. Before this exponential decay the time evolution of the magnetization obeys a power law $t^{-\beta/\nu z}$. All this universal scaling behaviour can be characterized by a set of three critical exponents, two static exponents β, ν and one dynamic exponent z.

Is there universal behaviour in the *short-time regime* of the dynamic evolution? For long, the answer had been no. It was believed that the behaviour of the dynamic systems in the short-time regime depends essentially on the microscopic details. However, it has recently been discovered that universal scaling behaviour emerges already in the *macroscopic* short-time regime, starting at a time just greater than a microscopic time scale t_{mic} [1]. Important is that extra critical exponents should be introduced to describe the dependence of the scaling behaviour on the initial conditions [1,2], or to characterize the scaling behaviour of special dynamic observables [3–5]. A typical dynamic process is that a magnetic system initially at high temperature with a small initial magnetization, is suddenly quenched to the critical temperature (without any external magnetic field) and then released to a time evolution with a dynamics of model A. A new dynamic exponent x_0 has been introduced to describe the scaling dimension of the initial magnetization. More surprisingly, at the beginning of the time evolution the magnetization undergoes a critical initial increase [1,6,7]

$$M(t) \sim m_0\, t^\theta \tag{1}$$

where θ is related to the scaling dimension x_0 of the initial magnetization m_0 by $\theta = (x_0 - \beta/\nu)/z$.

The physical background for the initial increase of the magnetization has not been completely clear. The critical initial increase has little to do with the symmetry breaking below the critical temperature. Actually similar phenomena can be observed even in case that the magnetization is not an order parameter. For the 6-state clock model and the XY model, below the Kosterlitz Thouless phase transition temperature no real long range order appears. The normal magnetization is not an order parameter. However, the power law initial increase is still observed in numerical simulations [8,9].

On the other hand, in recent years much attention has been drawn to statistical systems with frustration or quenched randomness. Critical behaviour of these systems is often quite different from that of regular systems. Due to the severe critical slowing down, numerical simulations of these systems are extremely difficult. Especially, our knowledge on the dynamic properties of these systems is poor.

In this paper, as a first approach to the short-time dynamics of statistical systems with frustrations, we investigate numerically the dynamic fully frustrated XY model below and at the Kosterlitz-Thouless phase transition temperature. We concentrate our attention on the scaling behaviour of the magnetization and its dependence on the initial value. Much effort is devoted to the understanding of the special properties induced by the sublattice

structure of the ground states. An investigation of the universal short-time behaviour of the dynamic systems is not only conceptually important, but also in the practical sense. Numerical simulations for the Ising and Potts model show that we may obtain already from the short-time dynamics the static critical exponents as well as the dynamic exponent z, which are normally defined and measured in equilibrium or in the long-time regime of the dynamic evolution [7,10,11,8,12,13]. Since our measurements in the short-time dynamics are always carried out at the beginning of the time evolution and the average is really a sample average rather than a time average based on the ergodicity assumption as in the measurements in equilibrium, the dynamic approach might be free of critical slowing down.

In the next section, the fully frustrated XY model is briefly introduced. In Sec. 3 and Sec. 4, numerical results are reported for the dynamic fully frustrated XY model. Finally we give some conclusions.

II. THE FULLY FRUSTRATED XY MODEL

The fully frustrated XY model in two dimensions (FFXY) can be defined by the Hamiltonian

$$H = K \sum_{<ij>} f_{ij} \ \vec{S}_i \cdot \vec{S}_j \ , \tag{2}$$

where $\vec{S}_i = (S_{i,x}, S_{i,y})$ is a planar unit vector at site i and the sum is over the nearest neighbours. In our notation the inverse temperature has been absorbed in the coupling K. Here f_{ij} takes the values $+1$ or -1, depending on the links. A simple realization of the FFXY model is defined by taking $f_{ij} = -1$ on half of the vertical links (negative links) while $+1$ on the others (positive links). This is shown in Fig. 1. The links marked by dotted lines represent the negative links.

In the FFXY model two phase transitions exist, the Kosterlitz-Thouless phase transition (XY-like) and the second order phase transition (Ising-like). This is very different from the regular XY model. Much effort has been made to locate the critical points for both transitions and measure the corresponding critical exponents. In a recent paper [14], it is reported that the XY-like phase transition temperature is $T_{KT} = 1/K_{KT} = 0.446$ while the Ising-like phase transition temperature $T_c = 1/K_c = 0.452$. These two measured values for the phase transition temperature are slightly different. Earlier results for the FFXY model and its ordering dynamics can be found in references [15–20].

One of the most important properties of the fully frustrated XY model is the sublattice structure of its ground states. In the regular XY model, in the ground state all spins orient in the same direction. However, for the FFXY model the lattice should be divided into four sublattices. All spins in each sublattice orient in the same direction, but the directions for the four sublattices are different and connected in a certain way, as it is shown in Fig. 1. For the whole lattice, the ground state preserves the global O(2) symmetry at any temperature, i.e. spins can rotate *globally*. No real long range XY-like order emerges in the FFXY model. This situation is similar as for the regular XY model. Besides the ground state shown in Fig. 1, there is another ground state which is just obtained by translating the configuration in Fig. 1 by one lattice spacing in y direction. Below the Ising-like critical temperature T_c, the Z_2 symmetry is broken. A second order phase transition occurs.

In this paper we study the short-time dynamic properties of the FFXY model below or at the XY-like phase transition temperature T_{KT}. Below the critical temperature T_{KT}, the FFXY model remains critical in the sense that the correlation length keeps divergent. Therefore, a scaling form is expected even below the critical temperature T_{KT}. However, the critical exponents may vary with respect to the temperature. Such a phenomenon has been observed in the 6-state clock model and the regular XY model [8,9]. The dynamic properties related to the Ising-like phase transition will not be discussed in this paper.

III. SUBLATTICE STRUCTURE OF DYNAMIC EVOLUTION

Let us consider a dynamic relaxation process starting from an initial state with a very high temperature and small magnetization [1]. As a direct generalization of the XY model, the magnetization for the FFXY model may also be defined as

$$\vec{M}(t) = \frac{1}{L^2} \sum_i \vec{S}_i \tag{3}$$

with L being the lattice size. As in the XY model, the magnetization here is also not an order parameter. To achieve an initial magnetization, we introduce an initial external magnetic field, e.g. in the x direction, as in the numerical simulation of the XY model [9]. Taking into account that the initial state is at a very high temperature, the initial Hamiltonian can be written as

$$H_0 = 2h \sum_i S_{i,x}. \tag{4}$$

To prepare the initial state, we update the system described by the initial Hamiltonian H_0 until it reaches equilibrium. Then the generated configurations of this initial system are used as initial configurations of the dynamic system. The initial magnetization generated is

$$\vec{M}(0) = (m_0, 0) \approx (h, 0), \qquad h \to 0. \tag{5}$$

There are, of course, many other methods to generate an initial magnetization. However, it has been demonstrated that the universal behaviour does not depend on these microscopic details, i.e. how a magnetization is constructed [9]. Effects of the microscopic details of the initial configurations are swept away in almost one Monte Carlo time step.

After preparation of an initial configuration, the system is released to the dynamic evolution of model A below or at the XY-like transition temperature. In this paper, the Metropolis algorithm is mainly used. To confirm universality, however, some simulations are repeated with the heat-bath algorithm. We stop updating the dynamic system at 150 Monte Carlo time steps, and repeat the procedure with another initial configuration. The average is over the independent initial configurations as well as the random numbers. We have performed simulations with lattice sizes $L = 8$, 16, 32, 64 and 128. The total number of samples for the average is between 30 000 and 60 000, depending on lattice sizes, initial states and algorithms. Errors are estimated by dividing the samples into three or four groups.

In Fig. 2, the time evolution of the magnetization is displayed in double-log scale with a solid line for the lattice size $L = 64$ and the initial magnetization $m_0 = 0.02$. The temperature is taken to be $T = 0.400$, which is slightly below the XY-like transition temperature

$T_{KT} = 0.446$ given in reference [14] (or $T_{KT} = 0.440(2)$ in [19]). In the figure $M(t)$ is the x-component of the magnetization $\vec{M}(t)$. The y-component of the magnetization $\vec{M}(t)$ remains zero since the initial value is zero. From the figure we see that the magnetization indeed increases after some time steps. The universal power law behaviour becomes apparent after about $20 - 30$ Monte Carlo time steps. From the slope of the curve, one measures the exponent $\theta = 0.184(6)$. In this simulation a global uniform initial external magnetic field h has been applied to the whole lattice, or in other words, the initial magnetization density distribution is uniformly generated. We call this initial state *the global start*.

Does the sublattice structure of the ground state play some role in the dynamic evolution? In equilibrium, it is known that the XY susceptibility should be calculated separately for each sublattice since the orientations of the spins in different sublattices differ from each other. But further understanding of the sublattice structure in numerical simulations can not so easily be achieved due to the O(2) symmetry and large fluctuations. In the short-time dynamics, the situation is somewhat different. The O(2) symmetry is violated by the initial magnetization. One can really measure the time evolution of the magnetization for each sublattice shown in Fig. 1 separately. The results are also included in Fig. 2. The two upper dotted lines represent the time evolution of the magnetization for the two sublattices connected to the positive links while the lower two dotted lines are those for the two sublattices connected to the negative links. In is very interesting that for sublattices connected to the positive links the magnetization increases from the beginning while for sublattices connected to the negative links they drop significantly in the first time steps. However, after a certain number of time steps the magnetization tends in all cases to the *same* universal power law behaviour even though the magnitudes remain different for the sublattices on the positive links and the negative links.

What is the relation between the magnetizations on the positive links and the negative links? In Fig. 3, the ratio $r(t)$ of the magnetization averaged over two sublattices on the positive links and that on the negative links is plotted with a solid line. This ratio stabilizes to a constant very quickly within 10 time steps. Averaging this ratio in a time interval $[10, 150]$, we get $r = 2.4147(8)$. What is this ratio? In the ground state drawn in Fig. 1, the magnitude of the angles between spins on the positive links and the x axis is $\pi/8$, while that between spins on the negative links and the x axis is $3\pi/8$. The ratio r should be nothing but the ratio of the x-components of the spins on both the positive links and the negative links. We see this by calculating $r_{th} = \cos(\pi/8)/\cos(3\pi/8) \simeq 2.4142$. The consistence between r_{th} and the measured one $r = 2.4147(8)$ is remarkable.

For a better understanding of this point we now divide the lattice into *two* sublattices, the sublattice on the positive links and the one on the negative links. We have performed a simulation with different initial magnetizations for the two sublattices, m_{0p} and m_{0n} respectively, taking, for example, $m_{0p}/m_{0n} = r_{th}$ and keeping the global initial magnetization $m_0 = 0.02$. We call such an initial state *two sublattice start*. The time-dependent magnetizations with this initial condition are plotted in Fig. 4. The solid line is the global magnetization while the upper and lower dashed line represent those for sublattices on the positive links and negative links respectively. Now, the decline for the magnetization on the negative links has disappeared. The corresponding ratio $r(t)$ is plotted in Fig. 3 with the dotted line. It is a constant from almost the very beginning of the time evolution. The averaged value is $r = 2.4146(6)$. However, the time period for the magnetization to enter

the universal power law behaviour is again $20 - 30$, almost the same as that in Fig. 2.

Before going further we would like to mention the problem of the *sharp preparation* of the initial magnetization. If the lattice size is infinite, in each initial configuration generated by the initial Hamiltonian H_0 an exact value $(m_0, 0)$ of the initial magnetization $\vec{M}(0)$ is automatically achieved. However, in practice the lattice size is finite and the initial magnetization $\vec{M}(0)$ fluctuates around $(m_0, 0)$. This is a kind of extra finite size effect. It causes a problem in high precision measurements. In order to reduce this effect, a sharp preparation technique has been introduced [6,7,21]. How important the sharp preparation technique is depends on the initial magnetization m_0 and what kind of observables one measures. The smaller the initial magnetization m_0 is, the more important the sharp preparation technique becomes. In Fig. 4, the result for the time evolution of the magnetization with the sharp preparation technique has been plotted with the dotted line. The curve almost overlaps with that without the sharp preparation technique. This shows that the extra finite size effect here is already quite small for the lattice size $L = 64$. For simplicity, our simulations are always carried out with no sharp preparation of the initial magnetization.

Now we go a step further. From the numerical simulations shown in Fig. 2, 3 and 4, and the discussions above, we understood that the universal behaviour of the dynamic system has close relation with the structure of the ground states. If the initial state is a completely random state with zero initial magnetization, the probabilities for the magnetization to evolve to different directions are the same, the averaged magnetization remains zero. However, if a non-zero initial magnetization is given to a certain direction, the time dependent magnetization grows in this direction since the energy is in favour of it. To clarify this point, we start with an initial state which is even closer to the ground state. We give different orientations to the initial magnetizations for the *four* sublattices as shown in Fig. 1. All the magnitudes of the initial magnetizations are $m_0 = 0.02$. This initial state we call *four sublattice start*. The time evolution of the magnetizations for different sublattices are shown in Fig. 5. Here $M(t)$ is just the projection of the magnetization on the direction of the initial magnetization. The solid line and dotted line are the magnetizations for the sublattices on the positive links while the circles and crosses are those on the negative links. They collapse on a line and show completely the same universal behaviour.

In Table I, values for the critical exponent θ measured in a time interval $[40, 150]$ for the three different initial states are collected. Within the statistical errors they are consistent. In the next section we will come back to this point.

IV. UNIVERSALITY AND SCALING

In the numerical measurements of the critical exponent θ we should pay attention to two possible effects, the finite size effect and the finite m_0 effect. For the dynamic process discussed in the last section, there are two kinds of finite size effects. One is the extra finite size effect from the initial configurations. This extra finite size effect is closely related to the problem of the sharp preparation of the initial configurations and has been discussed in the last section.

Another kind of finite size effect is the normal finite size effect which takes place in a time scale $t_L \sim L^z$. Whenever the system evolves into this time regime, the magnetization will decay by an exponential law $\exp(-t/t_L)$. In order to see the normal finite size effect,

we have plotted in double-log scale the time evolution of the magnetization for the lattice sizes $L = 8$, 16, 32, 64 and 128 with initial magnetization $m_0 = 0.02$ in Fig. 6. The upper solid line is the time-dependent magnetization for $L = 64$, while the dotted lines are those for $L = 8$, 16, 32 and 128 respectively. The curves for $L = 64$ and $L = 128$ more or less overlap. The values for the critical exponent θ are $\theta = 0.181(5)$ and 0.182(3) for $L = 64$ and $L = 128$ respectively. Therefore we conclude the finite size effect here is already negligibly small for the lattice size $L = 64$.

Rigorously speaking, the critical exponent is defined in the limit $m_0 = 0$. However, it is practically only possible to perform the measurement with finite m_0. The exponent θ measured may show some dependence on the initial magnetization m_0. In general, a linear extrapolation to the limit of $m_0 = 0$ should be carried out [7,21]. For this purpose, we have performed another simulation for the lattice size $L = 64$ with an initial magnetization $m_0 = 0.01$. The time-dependent magnetization is also displayed with the lower solid line in Fig. 6. The exponent θ obtained for $m_0 = 0.02$ and $m_0 = 0.01$ are $\theta = 0.181(5)$ and 0.179(7) respectively. Within the statistical errors they cover each other. Since the dependence of the exponent θ on m_0 is already rather weak here, a linear extrapolation is not necessary. This is also the reason why the results with and without the sharp preparation of the initial magnetization are not so different. In the further discussions in this paper we will work mostly with $L = 64$ and $m_0 = 0.02$.

Is the power law scaling behaviour in Eq. (1) for the magnetization really universal? For example, can it depend on the microscopic details of the initial state, the algorithms and the lattice types and even the additional non-nearest interactions and so on? Many discussions of this kind have recently been made [21,22,9,4,23]. Here we have also repeated some calculations with the heat-bath algorithm to confirm universality. The result for $L = 64$ and $m_0 = 0.01$ with the two sublattice start is plotted in Fig. 7 with the solid line. The initial magnetization m_{0p} and m_{0n} are given to the sublattices on the positive links and the negative links respectively, with $m_{0p}/m_{0n} = r_{th} = 2.4142$. The long dashed, dashed and dotted line are the results with the Metropolis algorithm with $m_0 = 0.02$ and the global start, two sublattice start and the four sublattice start respectively. All the measured values for the corresponding exponent θ are listed in Table I. The fact that all the four curves give consistent results for the exponent θ within the statistical errors provides strong support for universality. Especially the independence of the exponent θ on the initial states indicates that some physical mechanism closely related to the ground states essentially governs the time evolution of the dynamic systems.

To understand universality in the short-time dynamics, we keep in mind that there are two very different time scales in the dynamic systems, the microscopic time scale and the macroscopic time scale. A typical macroscopic time scale is t_τ or t_L. Universal behaviour emerges only after a sufficiently long time period in the microscopic sense. The time period which the dynamic system needs to sweep away the microscopic behaviour is called t_{mic}. One expects that the time scale t_{mic} is still very short in the macroscopic sense. In numerical simulations, a Monte Carlo time step can be considered as a typical microscopic unit. Most of the numerical simulations for dynamic systems show that $t_{mic} \sim 10 - 50$. In Fig. 7 we see that this is also the case for the FFXY model. These results are reasonable. Compared with the typical macroscopic time scale t_τ ot t_L, the microscopic time scale t_{mic} observed in numerical simulations is indeed very small. In some cases, universal behaviour emerges

actually already in one Monte Carlo time step, e.g. in the numerical measurement of the critical exponent θ for the two-dimensional Potts model [7,21]. Such a clean behaviour in the very short-time regime is somehow unexpected.

It is well known that for the XY-like phase transition no real long order emerges even below the transition temperature T_{KT}. The system remains critical in the sense that the correlation length is divergent. A similar scaling behaviour is expected for any temperature below T_{KT}. However, the critical exponents may vary with respect to the temperature. In Fig. 8, the time evolution of the magnetization for different temperatures has been displayed. We clearly see that there exists power law behaviour for all the temperatures below T_{KT}. However, the critical exponent θ varies essentially as can be seen from the results given in Table II. The dependence of the critical exponent θ on the temperature in the FFXY model is qualitatively the same but stronger than that for the regular XY model [9]. As the temperature decreases, the exponent θ first increases and then slowly decreases. Around the XY-like transition temperature $T_{KT} = 0.446$ [14] (or 0.440(2) in reference [19]), the exponent θ becomes quite small. Therefore, the power law behaviour around the critical temperature T_{KT} is less prominent compared with that at the lower temperature. We have also performed some simulations with temperatures above T_{KT}. Since the correlation length is divergent *exponentially* when the temperature approaches the XY-like transition point from above, however, no rigorous information for the XY-like transition temperature T_{KT} could be obtained from our data. Further investigation along this direction is needed.

V. CONCLUSIONS

We have numerically simulated the dynamic relaxation process of the fully frustrated XY model (FFXY) in two dimensions starting from an initial state with a very high temperature and small initial magnetization. Special attention has been drawn to the sublattice structure of dynamic evolution induced by the ground state. Universal power law behaviour is found independently of the sublattice structure of the initial states. The critical exponent θ has been measured for different temperatures below T_{KT}. Universality has been further confirmed by carrying out the simulations with both the Metropolis and the heat-bath algorithm. Many important problems remain open in connection with the present paper, e.g. the short-time behaviour of the dynamic FFXY model with respect to the Ising-like phase transition or the determination of the critical point as well as other critical exponents from the short-time dynamics.

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TABLES

	Metropolis			Heatbath
	I	II	III	II
θ	.184(6)	.182(5)	.181(5)	.186(6)

TABLE I. The exponent θ measured for lattice size $L = 64$ with different types of initial configurations and algorithms. I, II and III represent initial states of global start, two sublattice start and four sublattice start.

T	0.446	0.440	0.420	0.400	0.350	0.300	0.250
θ	.060(7)	. 079(4)	.141(5)	.181(5)	.245(3)	.263(2)	.260(2)

TABLE II. The exponent θ measured for different temperatures with the Metropolis algorithm. The lattice size is $L = 64$.

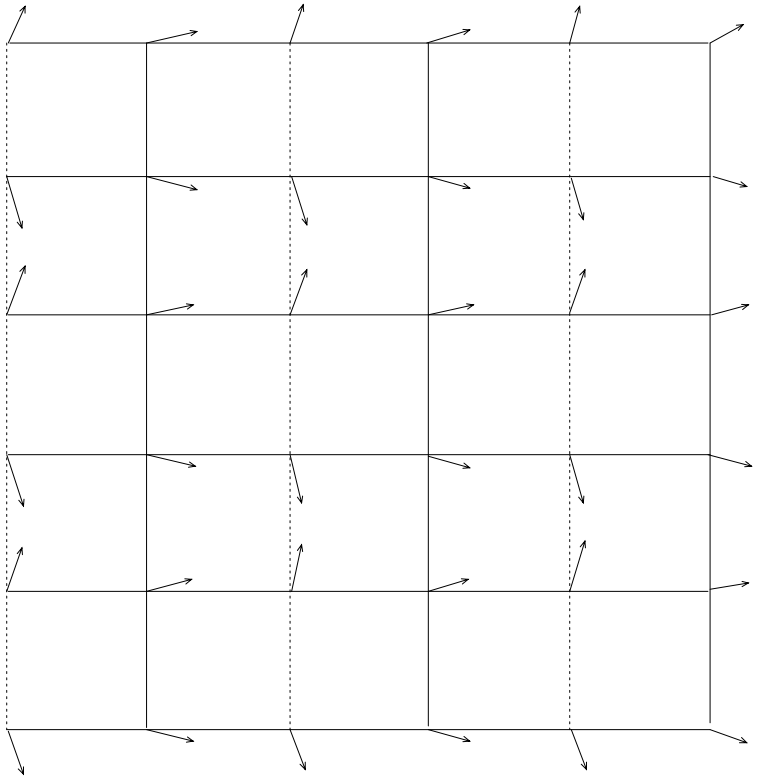

FIG. 1. One of the ground states for the FFXY model.

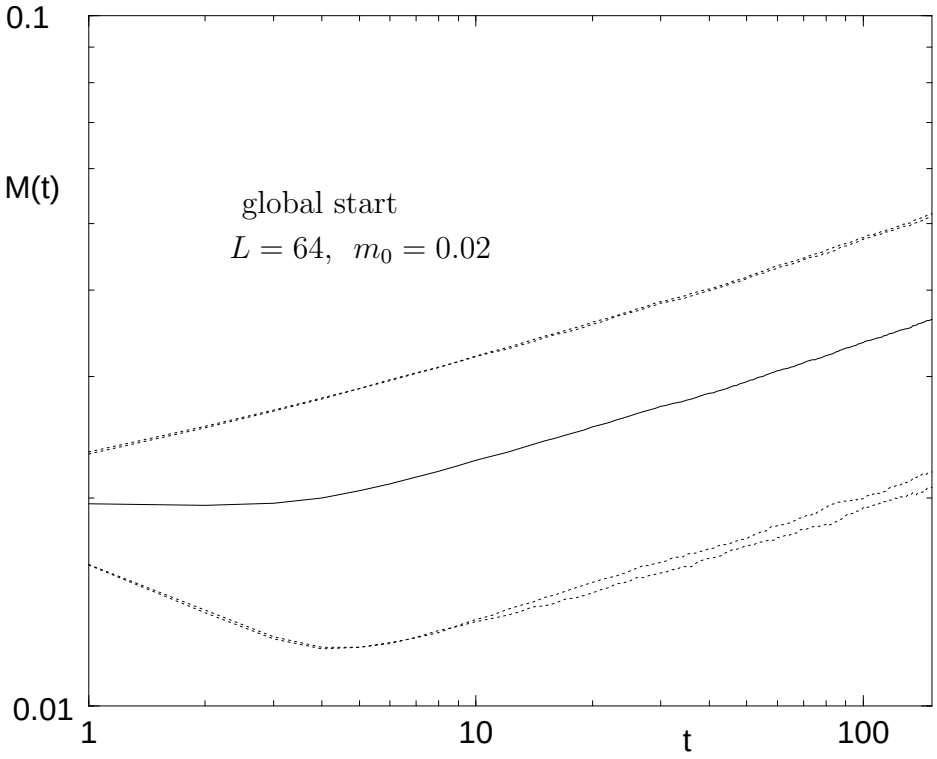

FIG. 2. The time evolution of the magnetization with the global start for $L = 64$ and $m_0 = 0.02$ with the Metropolis algorithm is plotted in double-log scale. $M(t)$ is the x-component of the magnetization $\vec{M}(t)$. The solid line represents the global magnetization while dotted lines are those for the four sublattices.

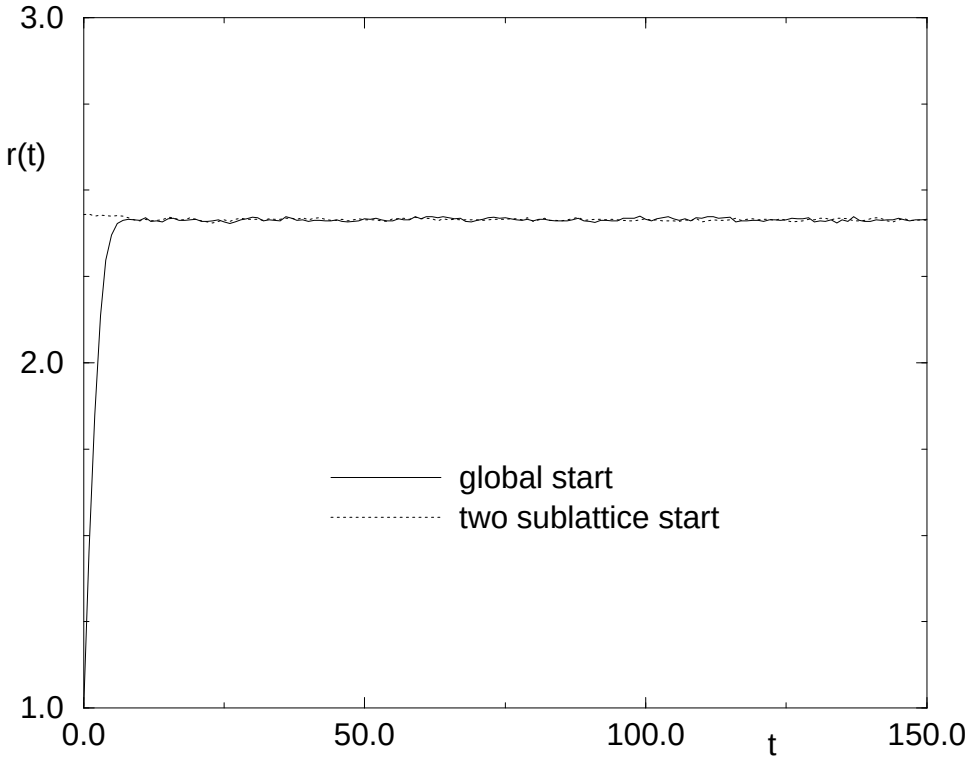

FIG. 3. The ratio $r(t)$ for different initial states.

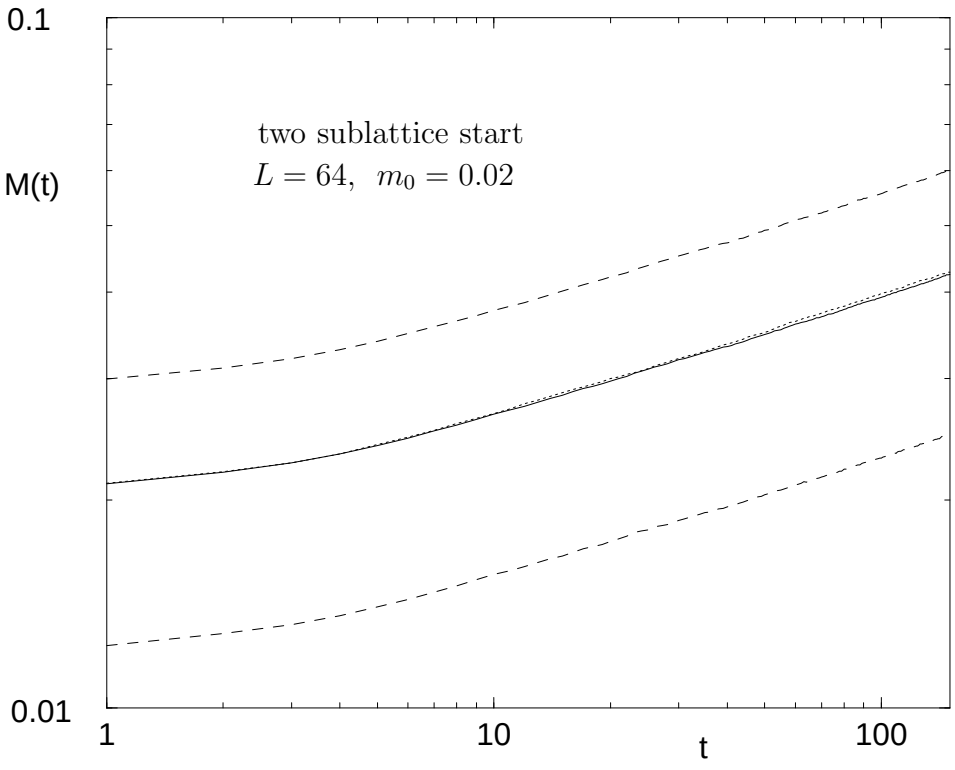

FIG. 4. The time evolution of the magnetization with the two sublattice start for $L = 64$ and $m_0 = 0.02$ with the Metropolis algorithm is plotted in double-log scale. $M(t)$ is the x-component of the magnetization $\vec{M}(t)$. The solid line represents the global magnetization while dashed lines are those for the sublattices. For comparison, the dotted line is the global magnetization with the sharp preparation of the initial magnetizations.

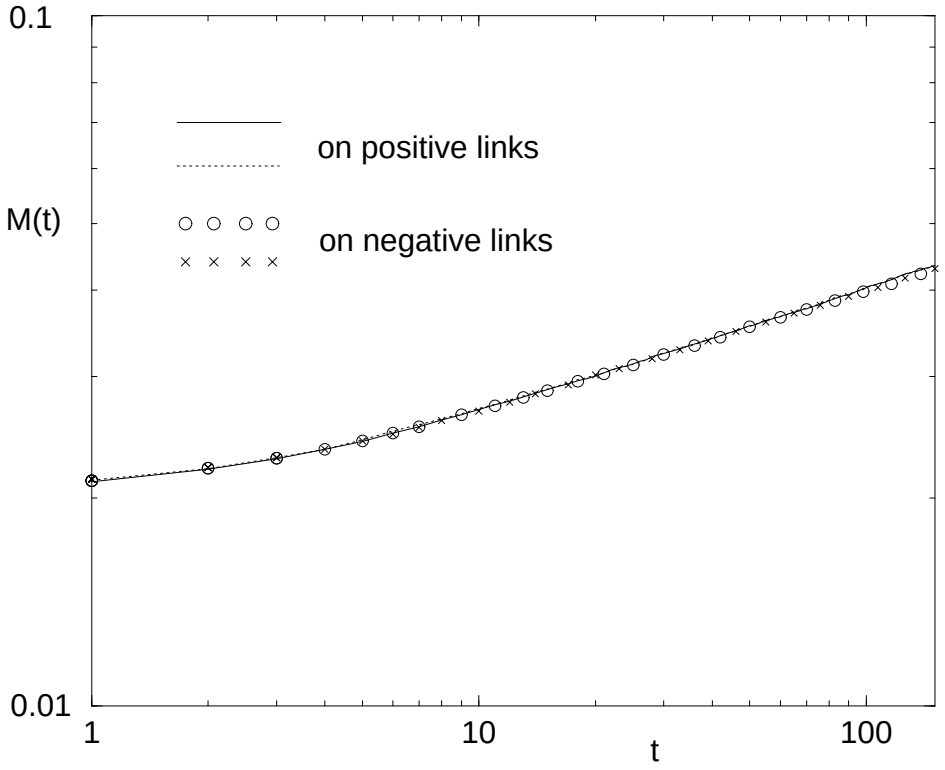

FIG. 5. The time evolution of the magnetization with the four sublattice start for $L = 64$ and $m_0 = 0.02$ with the Metropolis algorithm is plotted in double-log scale. $M(t)$ is the projection of the magnetization $\vec{M}(t)$ on the initial direction. The solid and dotted line are the magnetizations for the sublattices on the positive links while the circles and crosses represent those on the negative links.

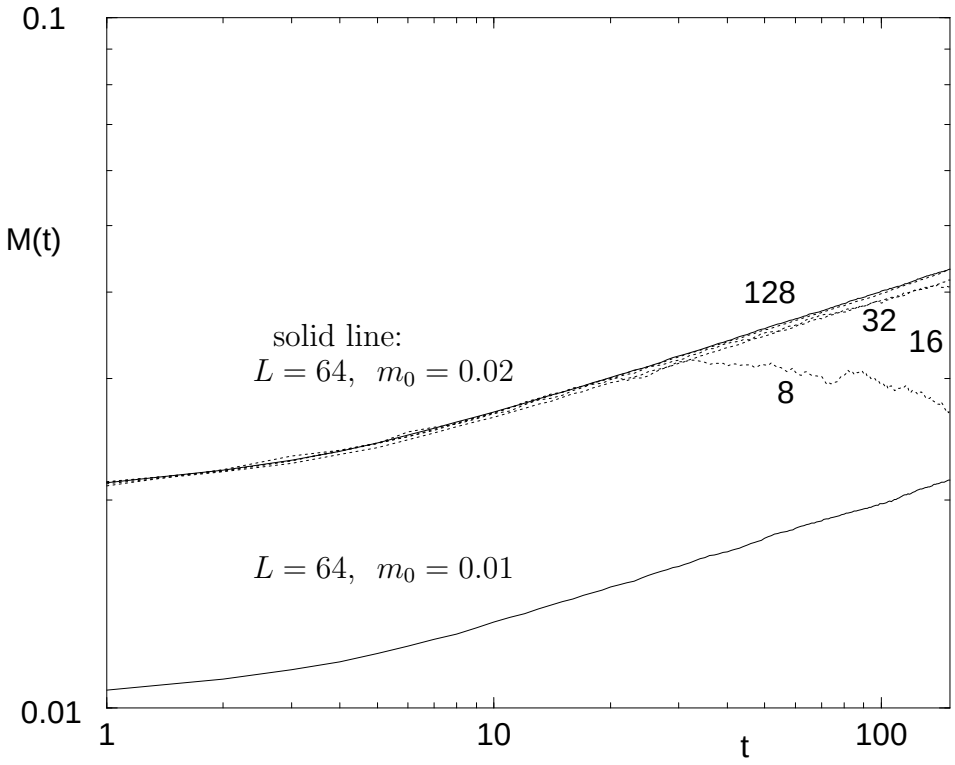

FIG. 6. The time evolution of the magnetization with the four sublattice start for different L and m_0 with the Metropolis algorithm is plotted in double-log scale. $M(t)$ is the projection of the magnetization $\vec{M}(t)$ on the initial direction. The solid line represents the magnetization for $L = 64$ while the dotted lines are those for other lattice sizes.

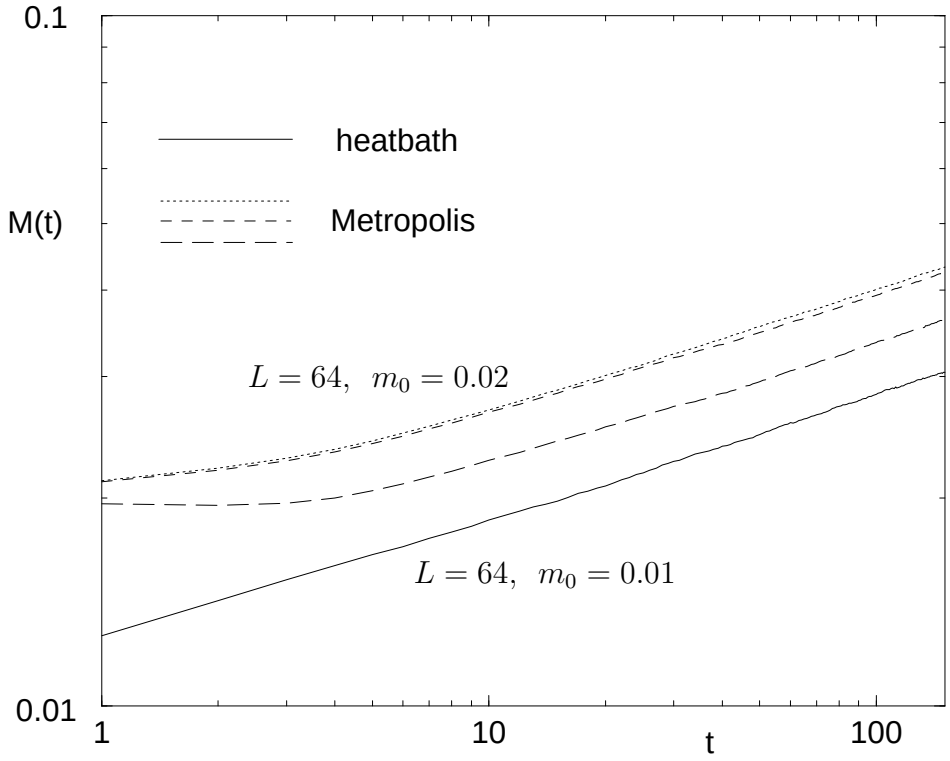

FIG. 7. The time evolution of the magnetization for different initial states and algorithms is plotted in double-log scale. $M(t)$ is the projection of the magnetization $\vec{M}(t)$ on the initial direction. The solid line represents the mag- netization for $L = 64$ and $m_0 = 0.01$ with the heat-bath algorithm and the two sublattice start while long dashed, dashed and dotted lines are those for $L = 64$ and $m_0 = 0.02$ with the Metropolis algorithm for the global, two sublattice and four sublattice start respectively.

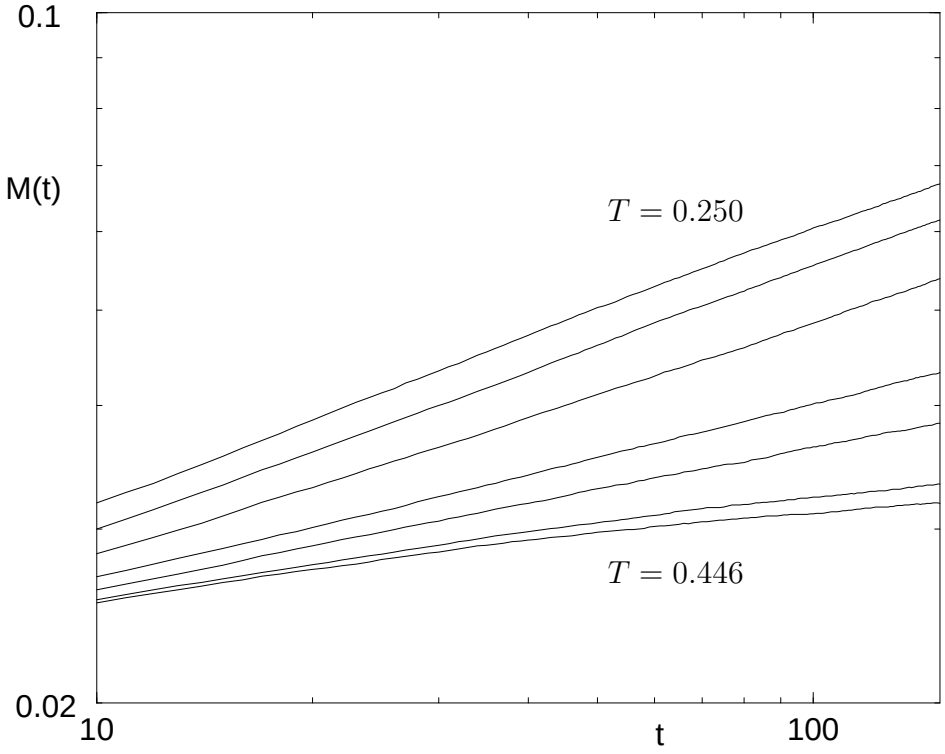

FIG. 8. The time evolution of the magnetization for $L = 64$ and $m_0 = 0.02$ with different temperatures is plotted in double-log scale. The four sublattice start and the Metropolis algorithm are used in the simulations. $M(t)$ is the projection of the magnetization $\vec{M}(t)$ on the initial direction. From above, the temperature is $T = 0.250$, 0.300, 0.350, 0.400, 0.420, 0.440 and 0.446 respectively.